

# Facile and efficient chloro-bridged Iridium(III) dimers as OLED materials: Opening up new possibilities

*Michael.Y. Wong,<sup>a</sup> Guohua Xie,<sup>b</sup> Clarisse. Tourbillon,<sup>c,d</sup> Martina Sandroni,<sup>c,e</sup> David B. Cordes,<sup>a</sup>  
Alexandra M. Z. Slawin,<sup>a</sup> Ifor D. W. Samuel,<sup>b</sup> Eli Zysman-Colman<sup>\*a</sup>*

<sup>a</sup> EaStCHEM School of Chemistry, University of St Andrews, St Andrews, Fife, UK, KY16 9ST, Fax: +44-1334 463808; Tel: +44-1334 463826; E-mail: [eli.zysman-colman@st-andrews.ac.uk](mailto:eli.zysman-colman@st-andrews.ac.uk);

<sup>b</sup> School of Physics and Astronomy, University of St. Andrews, North Haugh, St. Andrews, Fife, UK, KY16 9SS

<sup>c</sup> Département de Chimie, Université de Sherbrooke, Sherbrooke, Québec, Canada, J1K 2R1,

<sup>d</sup> Current address: Laboratoire PPSM - CNRS UMR 8531, ENS Cachan, 61 Av du Président Wilson, 94235 Cachan Cedex France

<sup>e</sup> Current address: CEMCA UMR CNRS 6521, Université de Bretagne Occidentale, 6 av. Victor Le Gorgeu, Brest, France, 29200

URL: <http://www.zysman-colman.com>

## SUPPORTING INFORMATION

### Table of contents:

|   | Pages   |
|---|---------|
| <sup>1</sup> H, and <sup>13</sup> C and NMR spectra   | S2-S10  |
| <sup>1</sup> H NMR spectra comparisons of individual C <sup>N</sup> ligands and the corresponding complexes | S11-S12 |
| Normalized absorption and emission spectra of individual complexes  | S13-S14 |
| Calculated absorption spectra for complexes <b>1a</b> and <b>2a</b>   | S15-S16 |
| Absorption and molar absorptivity data  | S16     |
| CV traces of individual complexes   | S17-S19 |

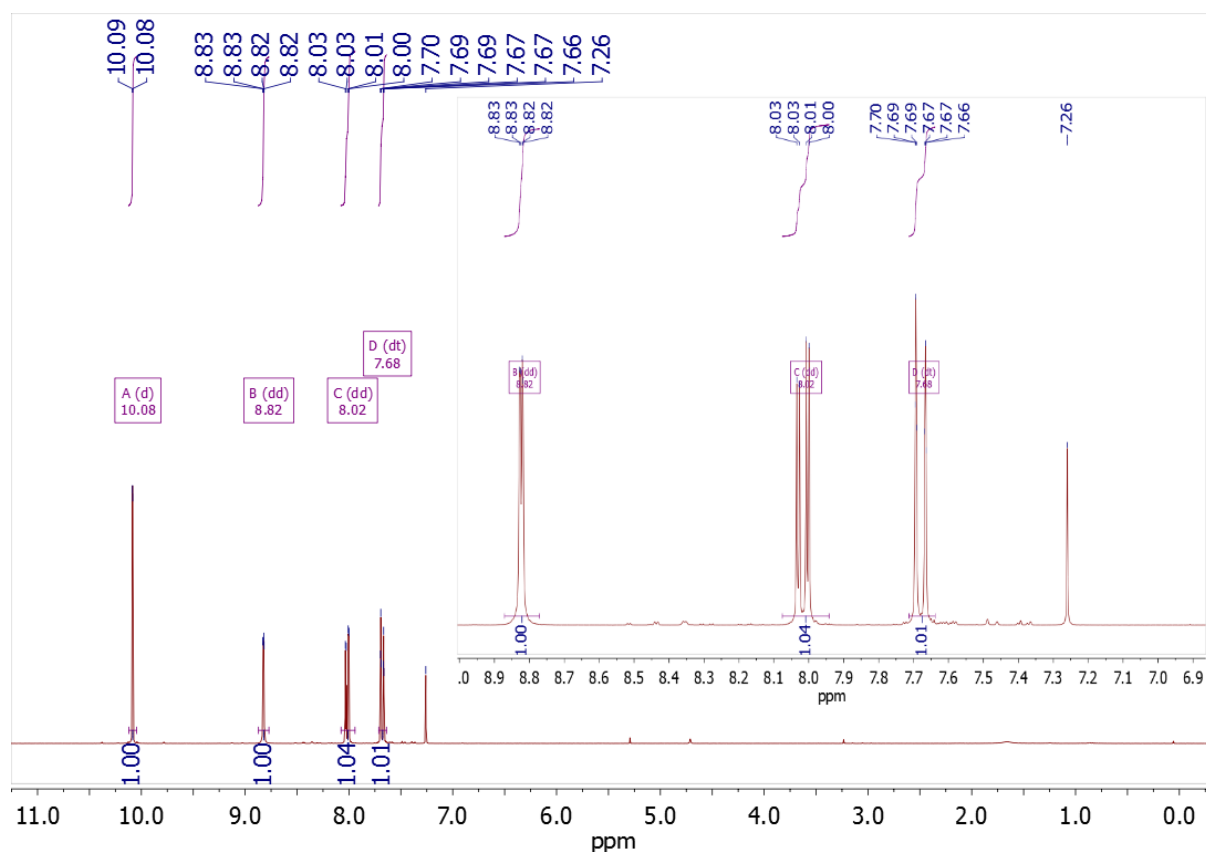


Figure S1. <sup>1</sup>H NMR of 2-bromo-5-formylpyridine.

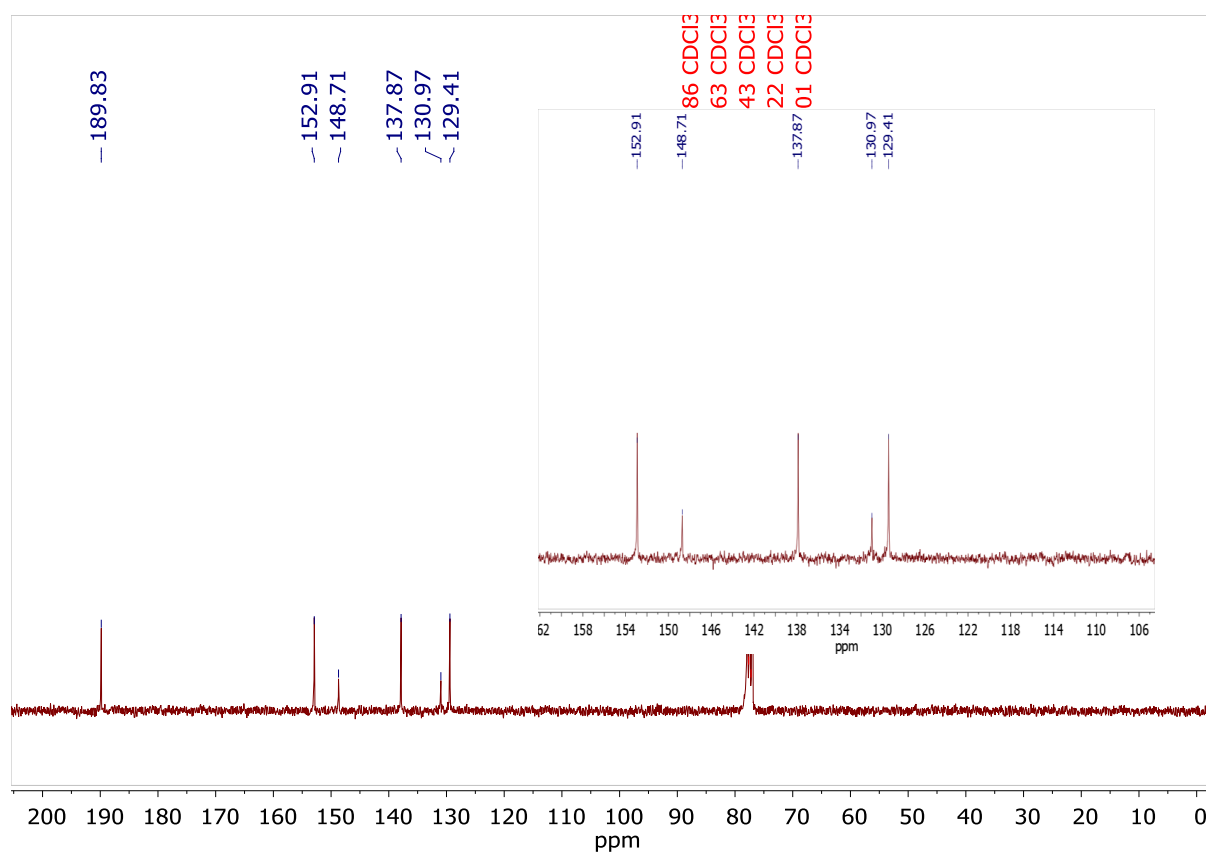


Figure S2. <sup>13</sup>C NMR of 2-bromo-5-formylpyridine.

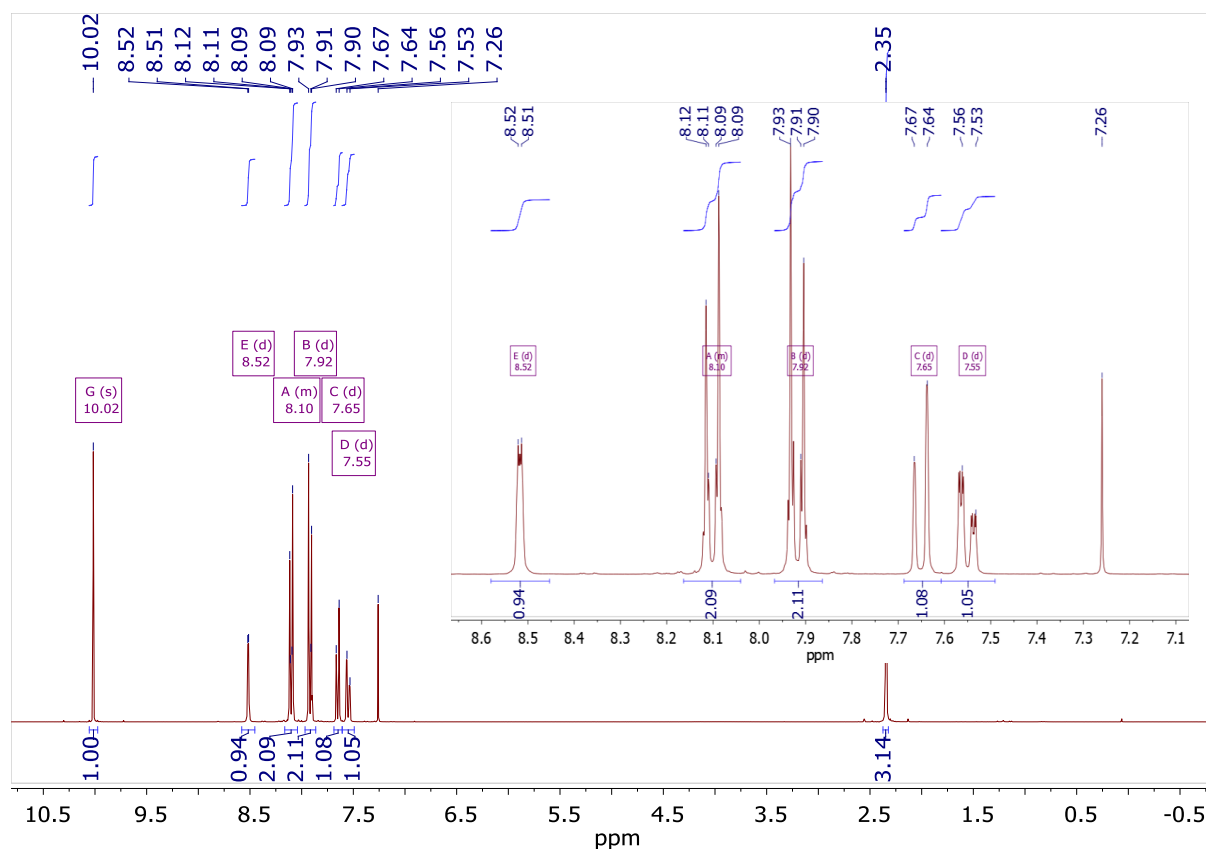


Figure S3. <sup>1</sup>H NMR of **4-CHO-mppy**.

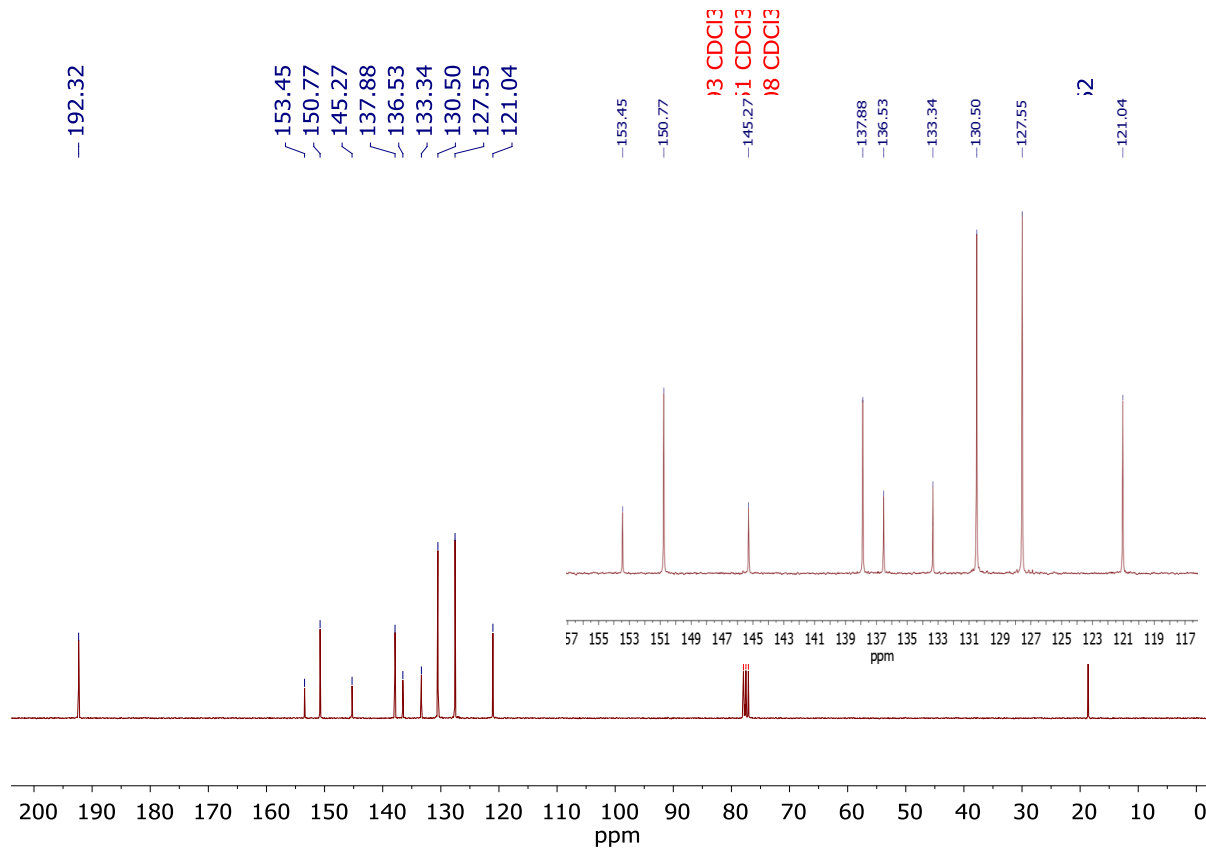


Figure S4. <sup>13</sup>C NMR of **4-CHO-mppy**.

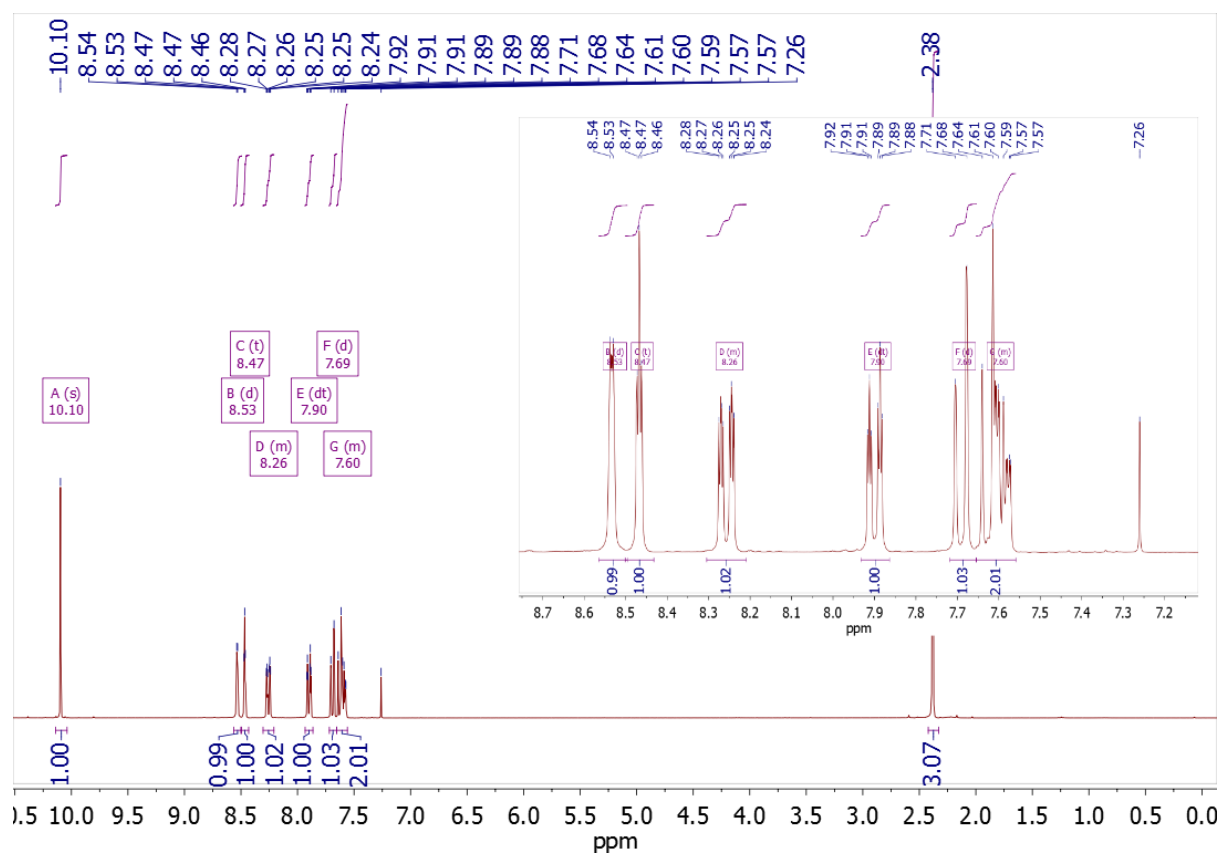


Figure S5. <sup>1</sup>H NMR of **3-CHO-mppy**.

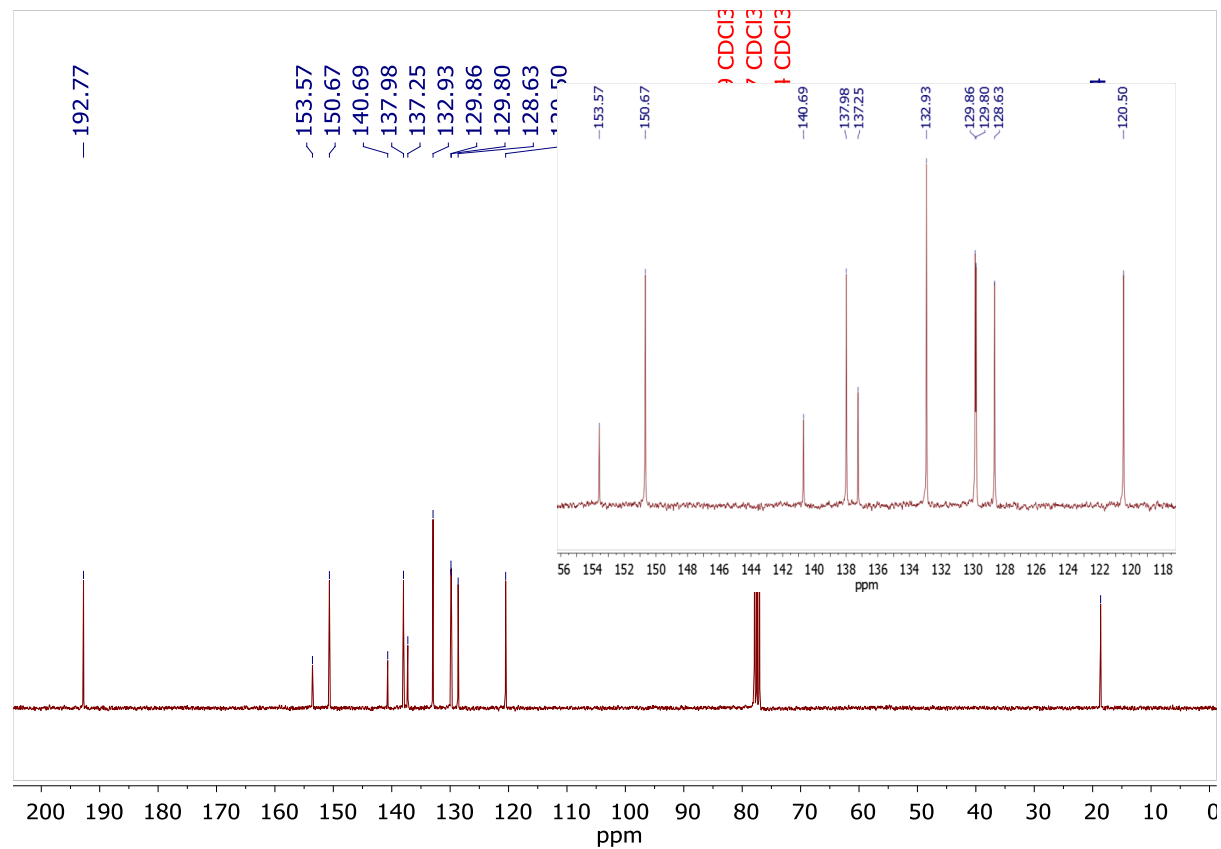


Figure S6. <sup>13</sup>C NMR of **3-CHO-mppy**.

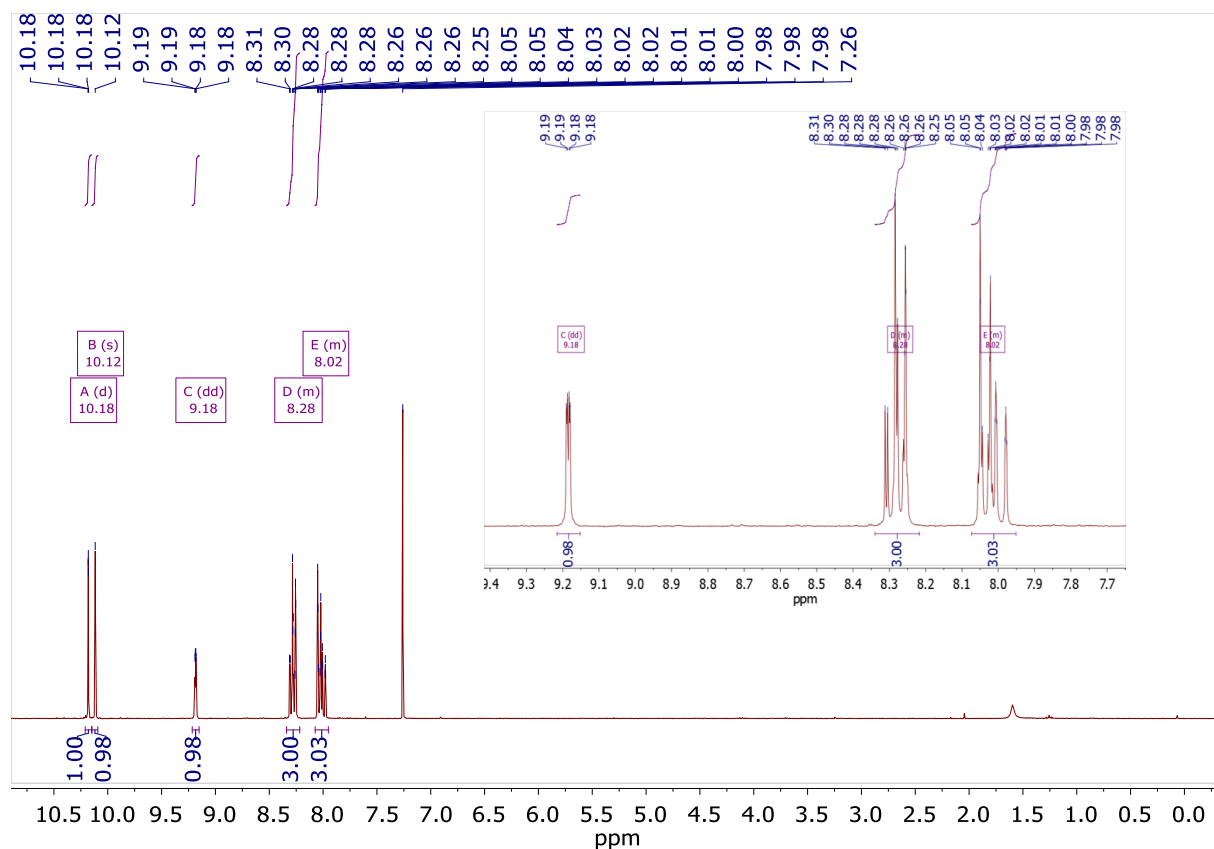


Figure S7. <sup>1</sup>H NMR of 4-CHO-fppy.

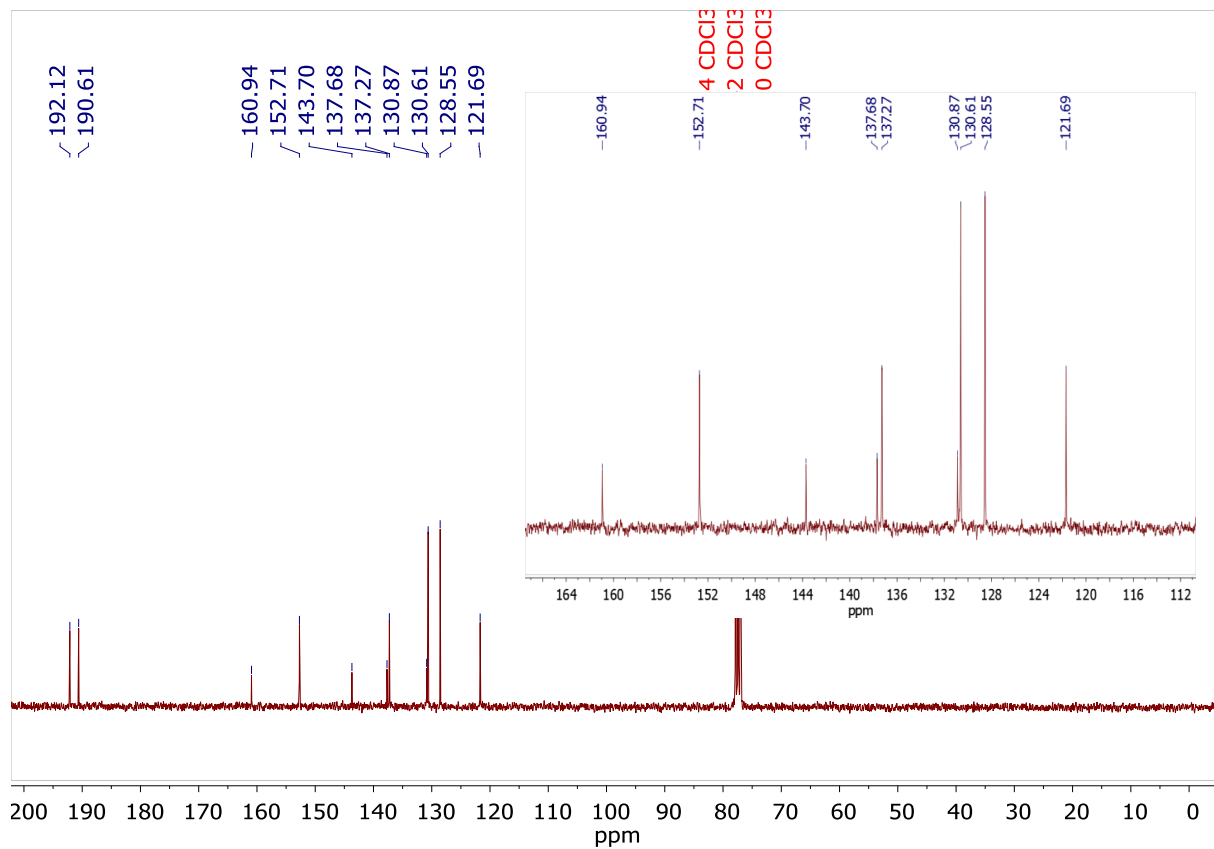


Figure S8. <sup>13</sup>C NMR of 4-CHO-fppy.

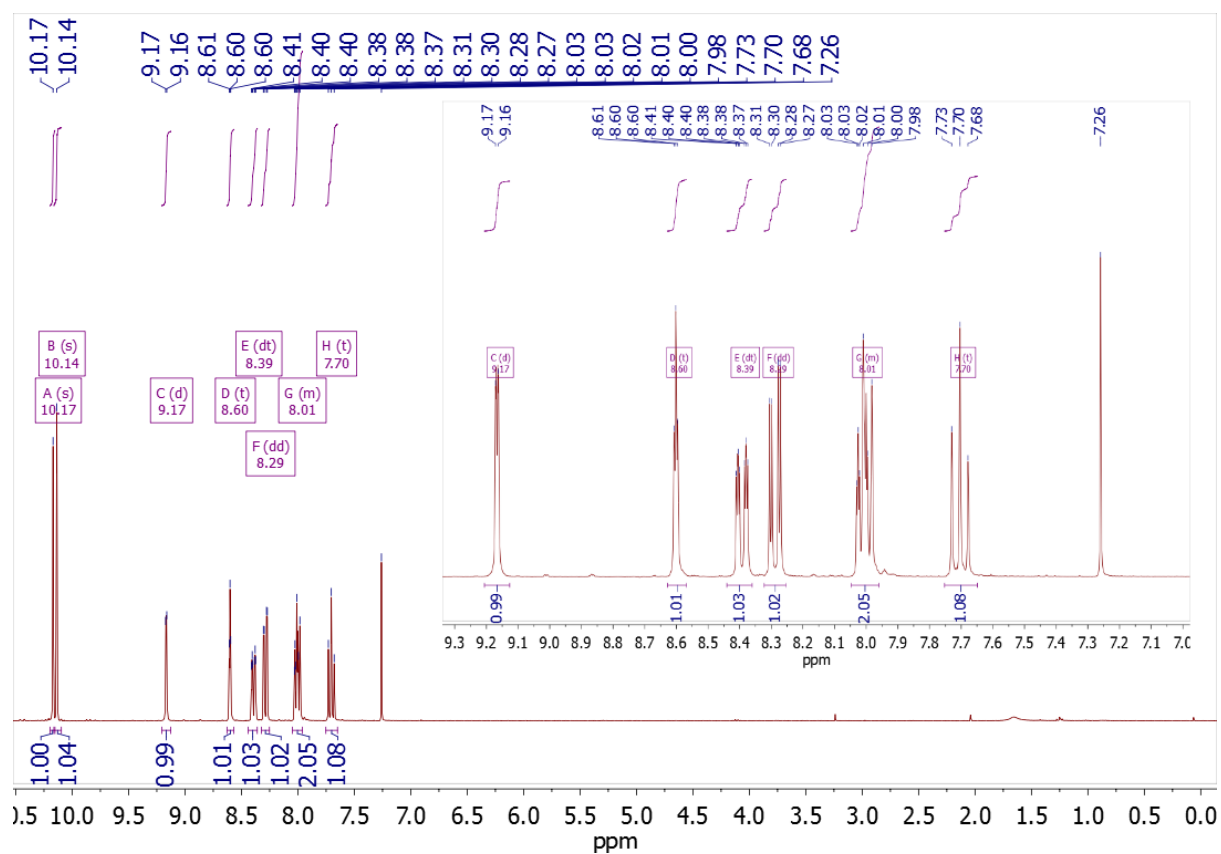


Figure S9. <sup>1</sup>H NMR of **3-CHO-fppy**.

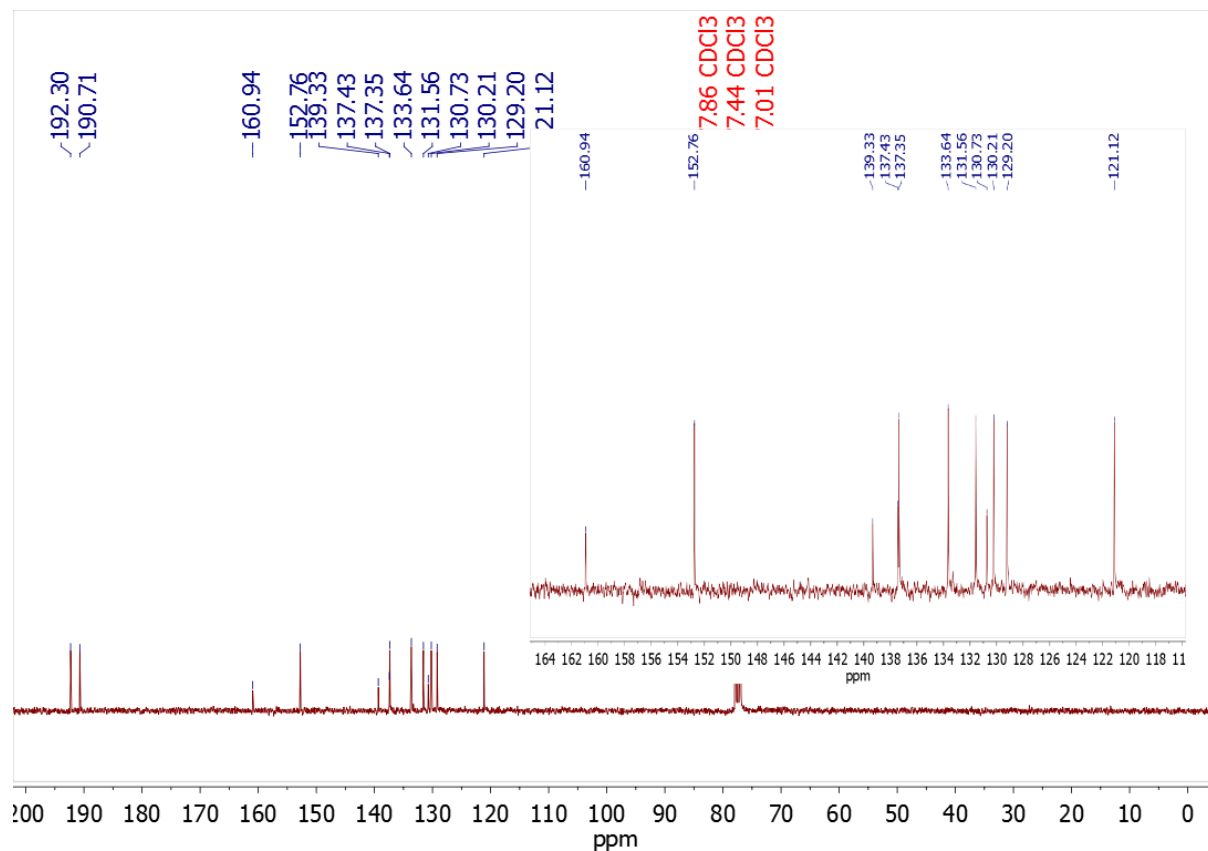


Figure S10. <sup>13</sup>C NMR of **3-CHO-fppy**.

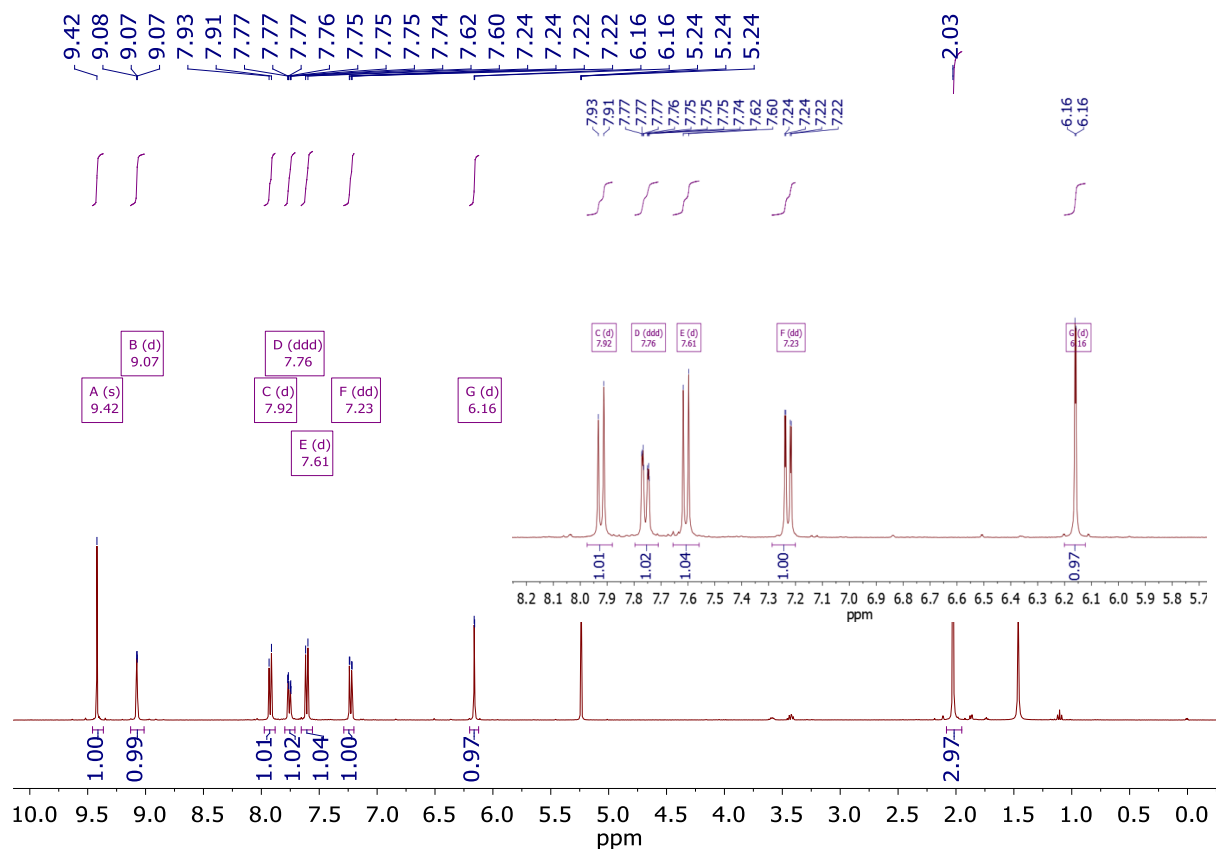


Figure S11. <sup>1</sup>H NMR of complex **1a**.

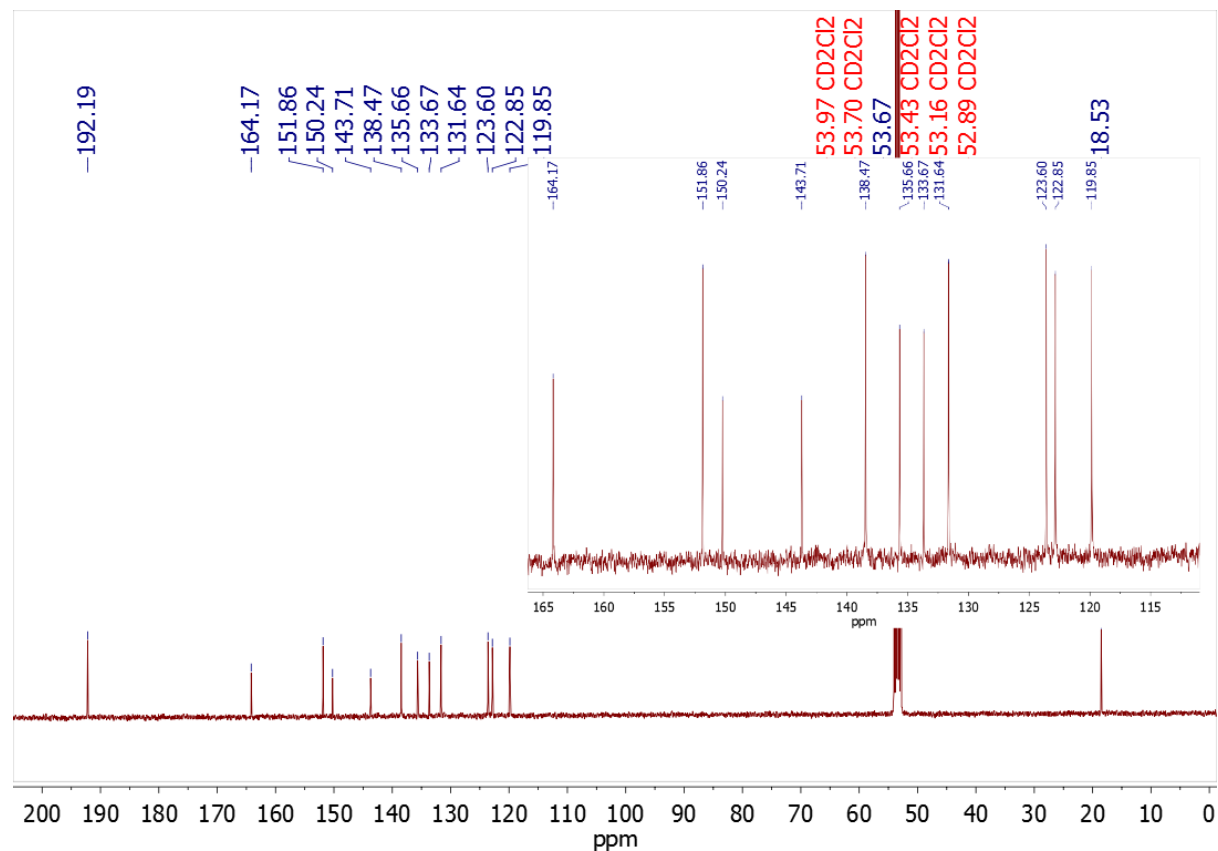


Figure S12. <sup>13</sup>C NMR of complex **1a**.

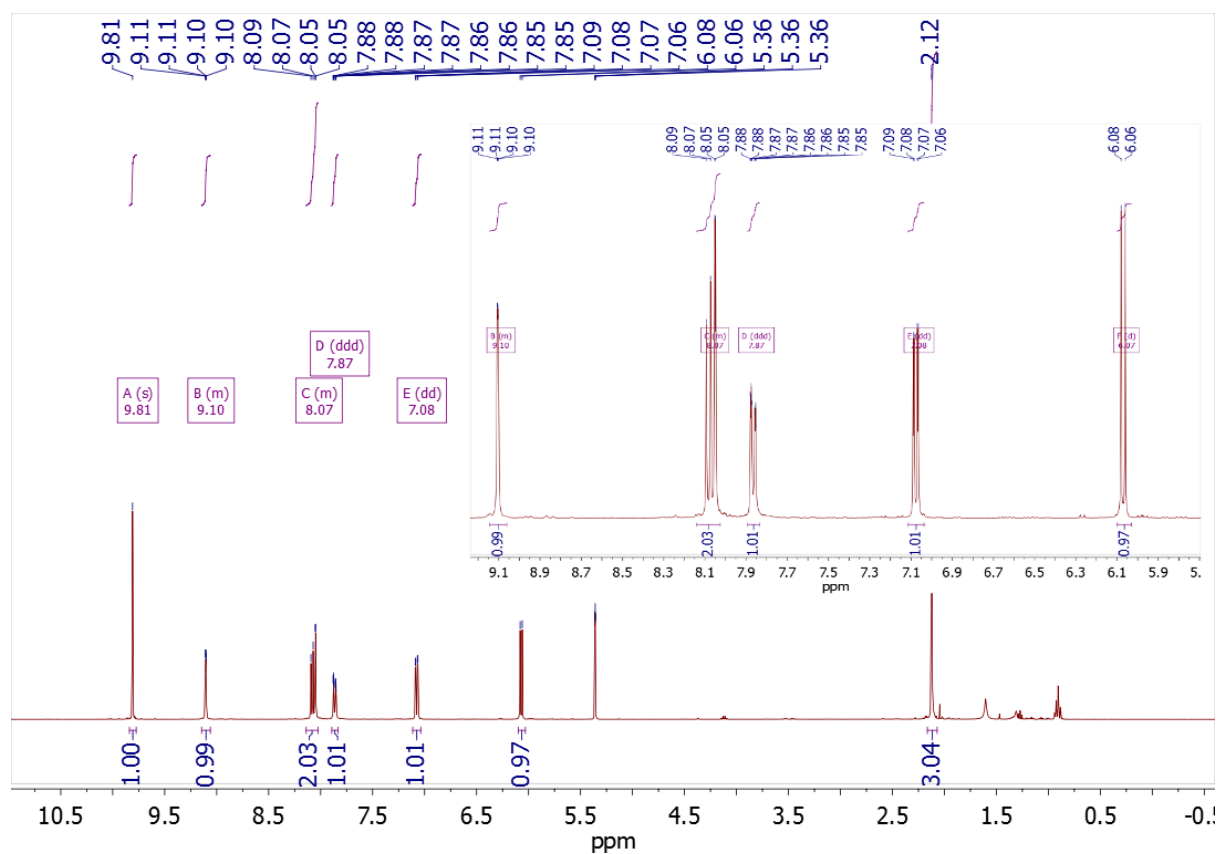


Figure S13. <sup>1</sup>H NMR of complex **1b**.

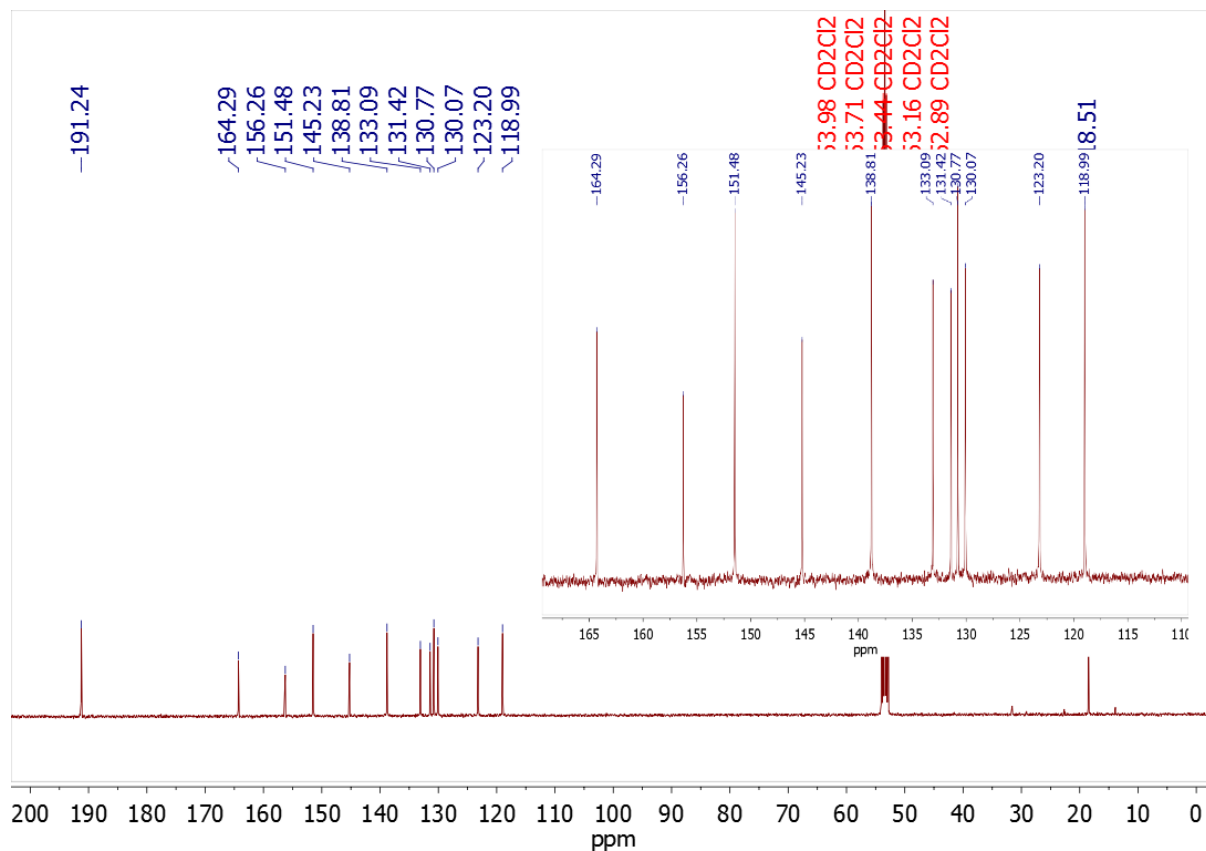


Figure S14. <sup>13</sup>C NMR of complex **1b**.



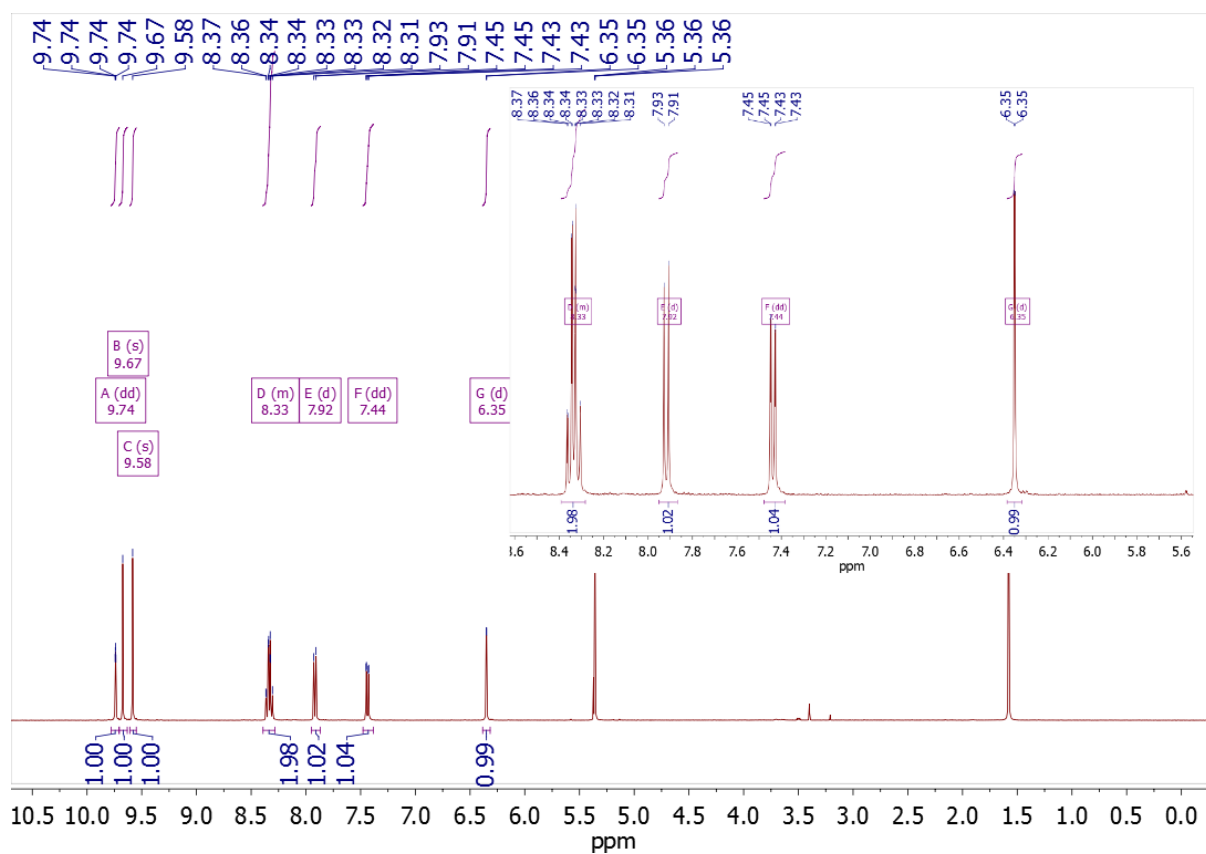


Figure S15.  $^1\text{H}$  NMR of complex **2a**.

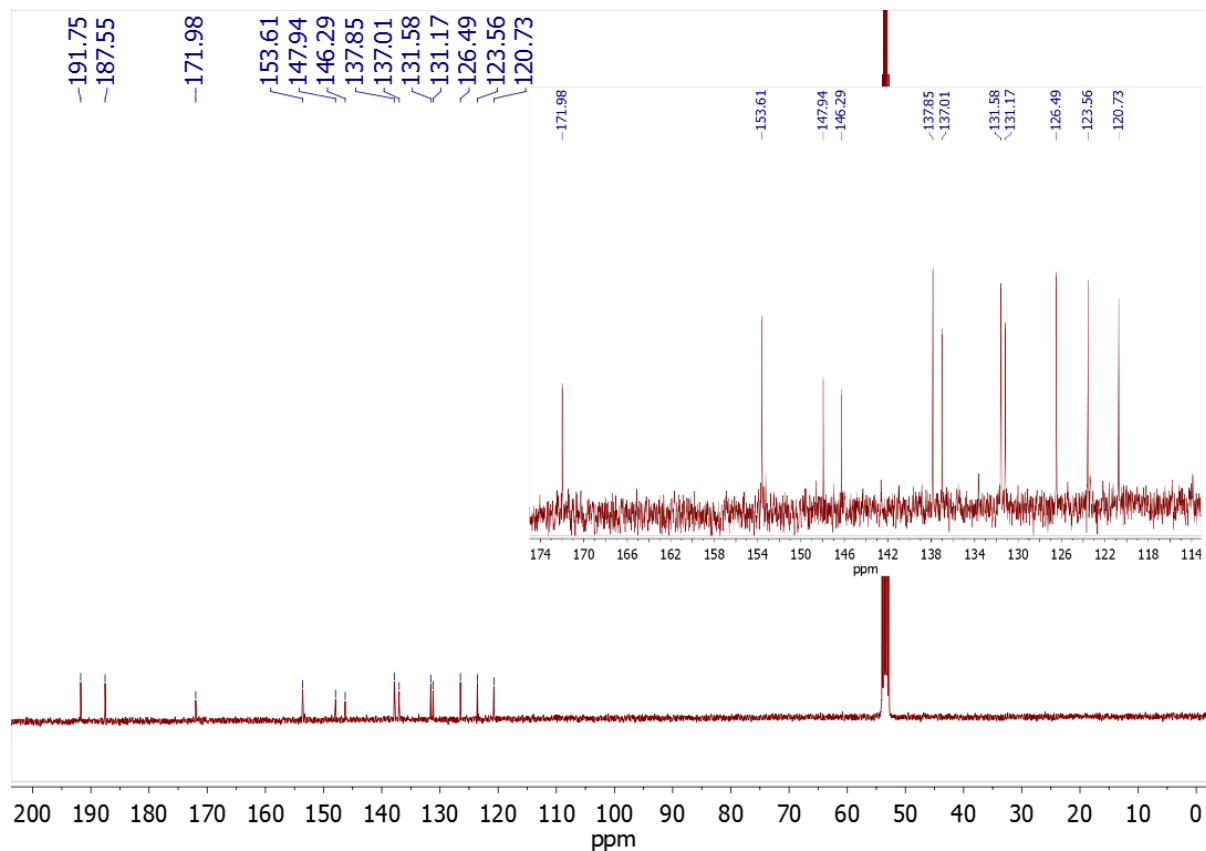


Figure S16.  $^{13}\text{C}$  NMR of complex **2a**.

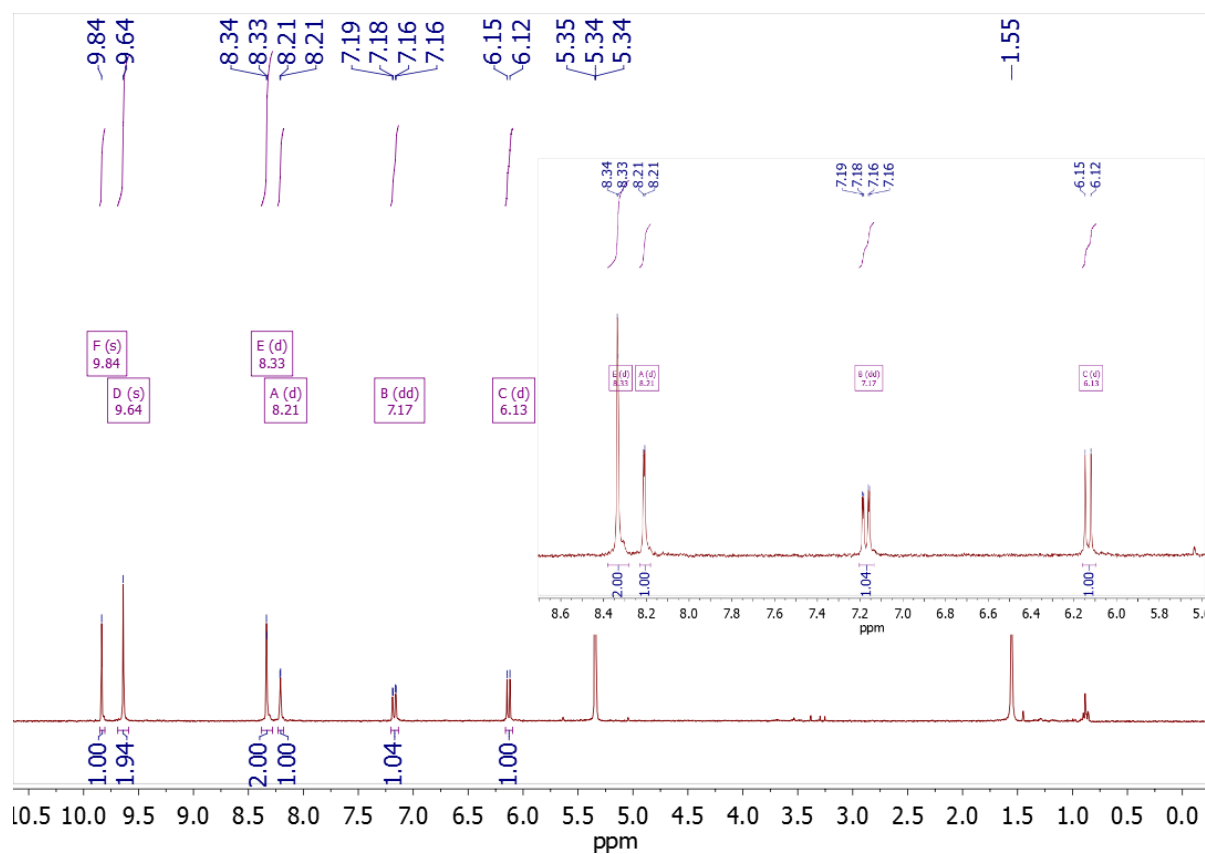


Figure S17.  $^1\text{H}$  NMR of complex **2b**.

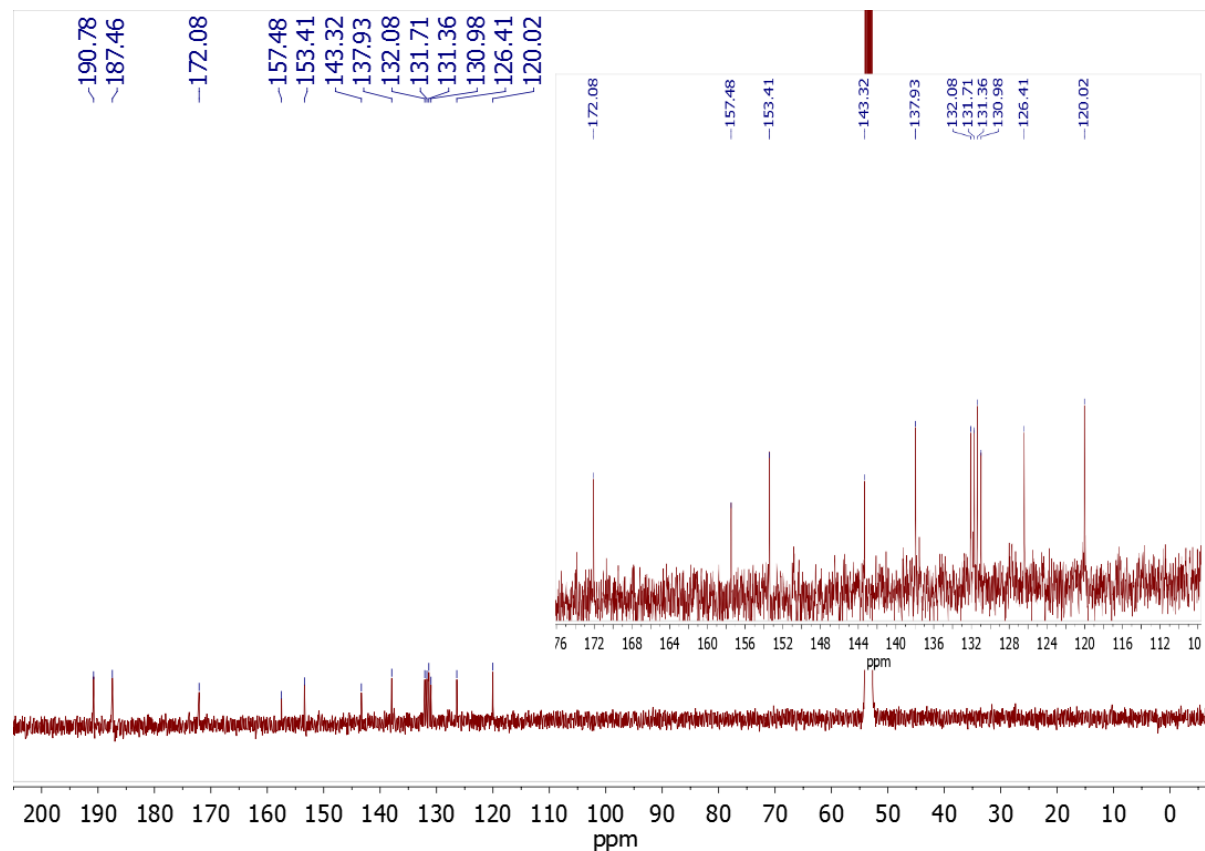


Figure S18.  $^{13}\text{C}$  NMR of complex **2b**.

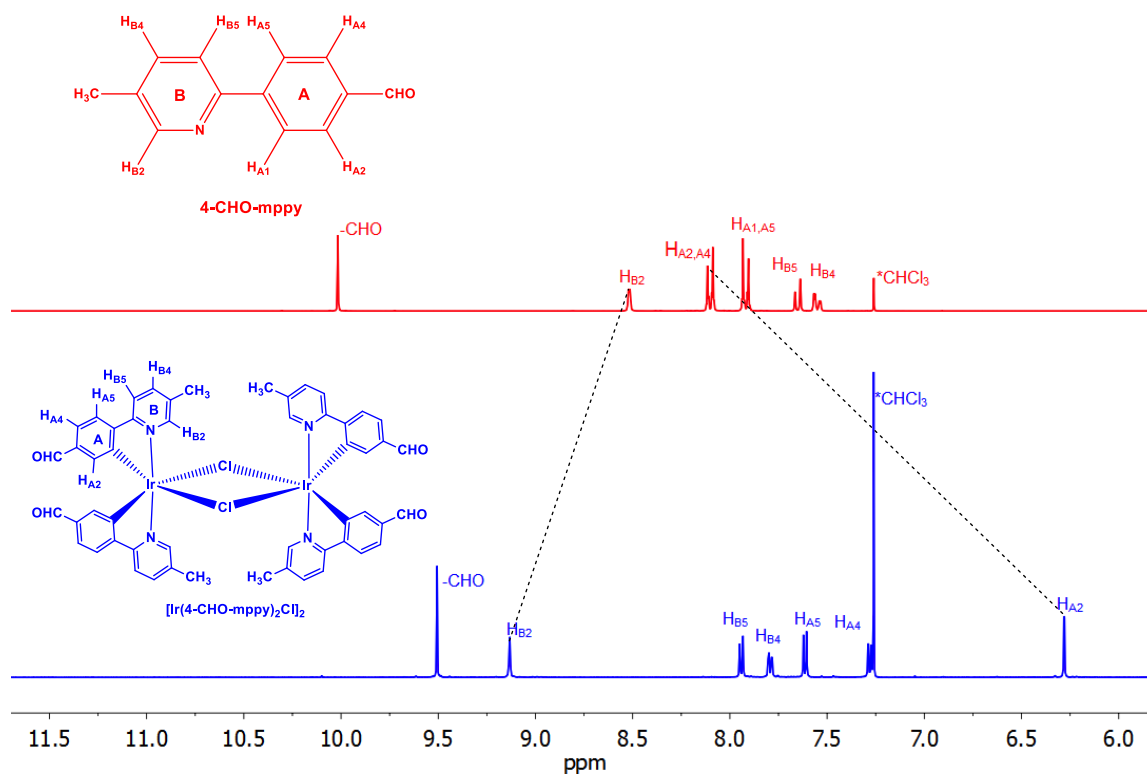


Figure S19. Comparison of  $^1\text{H}$  NMR between **4-CHO-mppy** and complex **1a**.

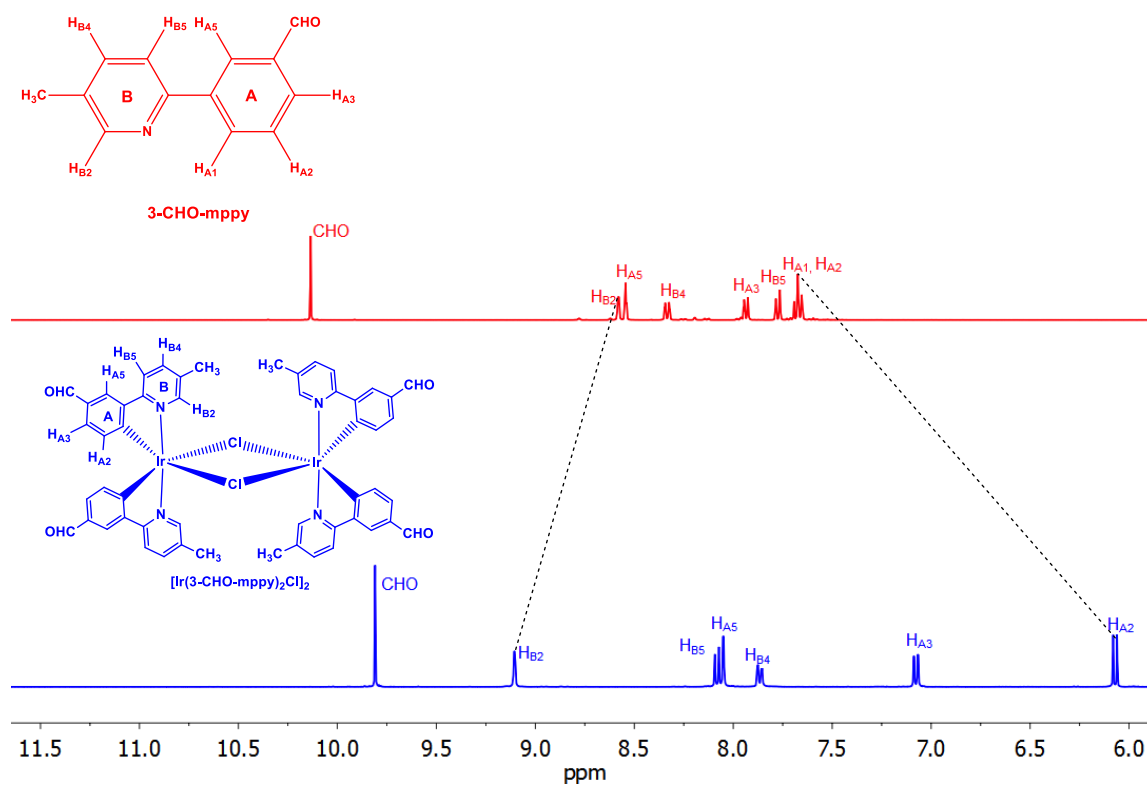


Figure S20. Comparison of  $^1\text{H}$  NMR between **3-CHO-mppy** and complex **1b**.

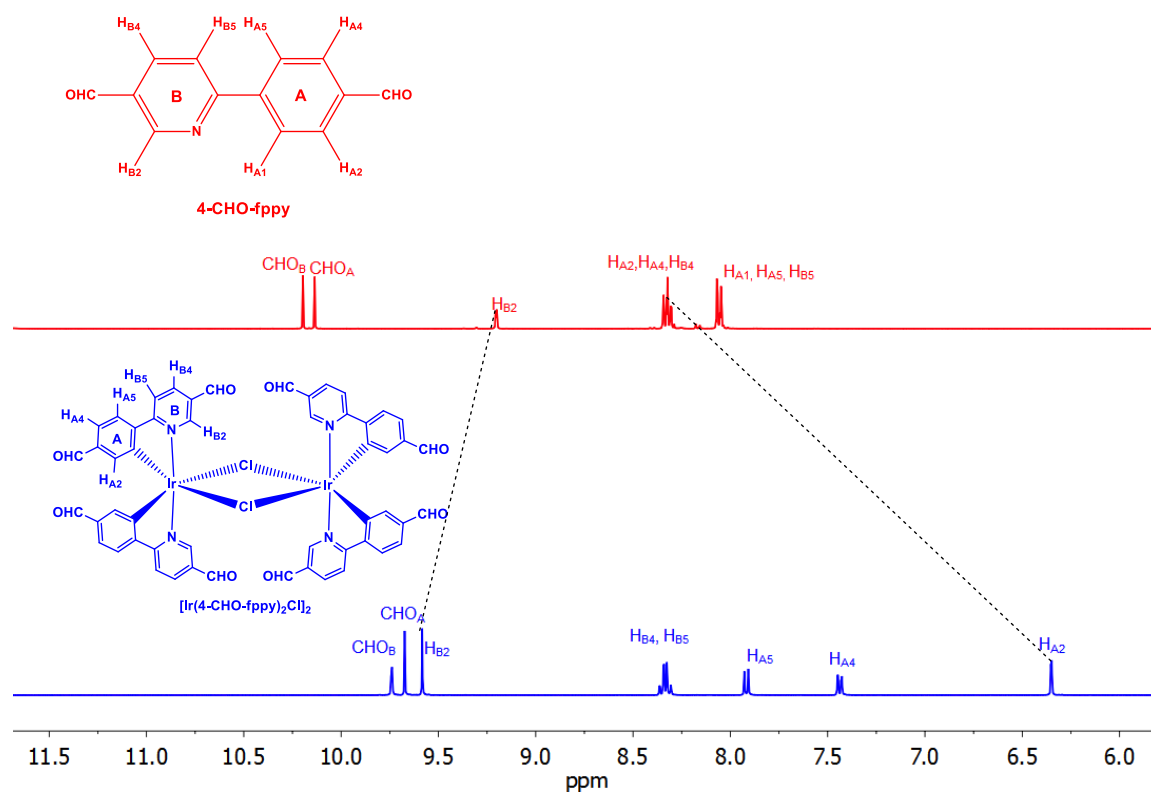


Figure S21. Comparison of  $^1\text{H}$  NMR between **4-CHO-fppy** and complex **2a**.

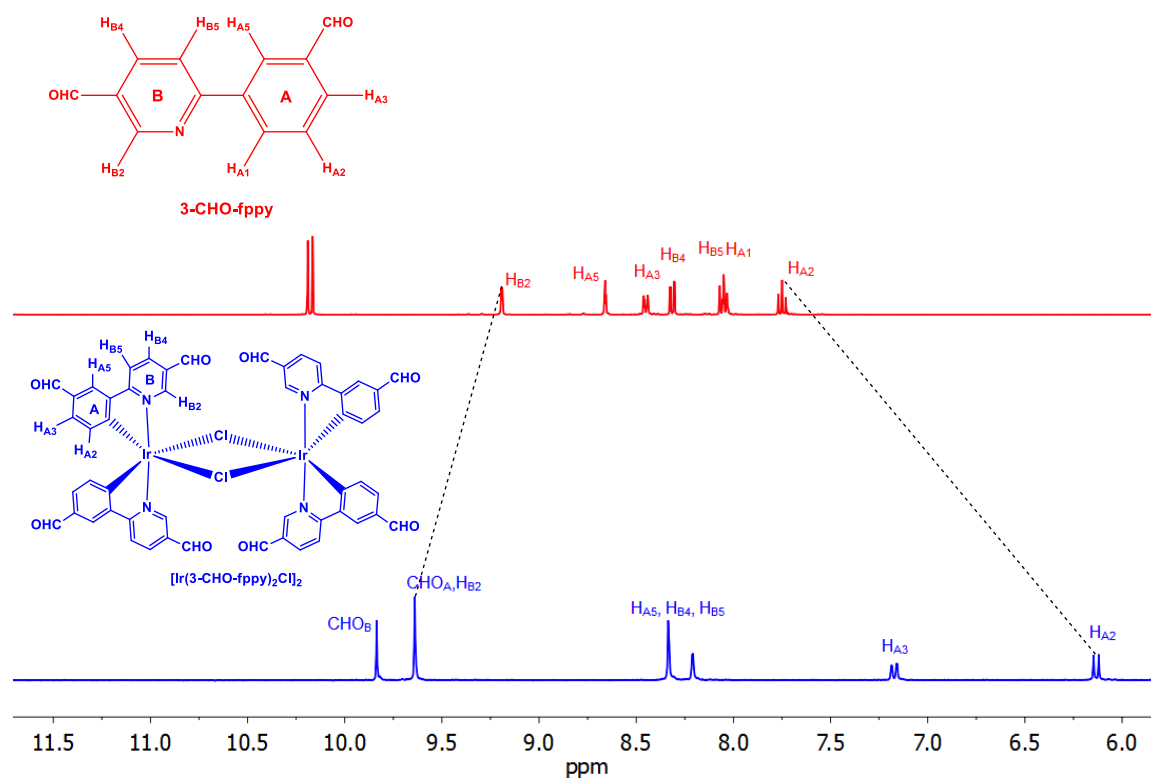


Figure S22. Comparison of  $^1\text{H}$  NMR between **3-CHO-fppy** and complex **2b**.

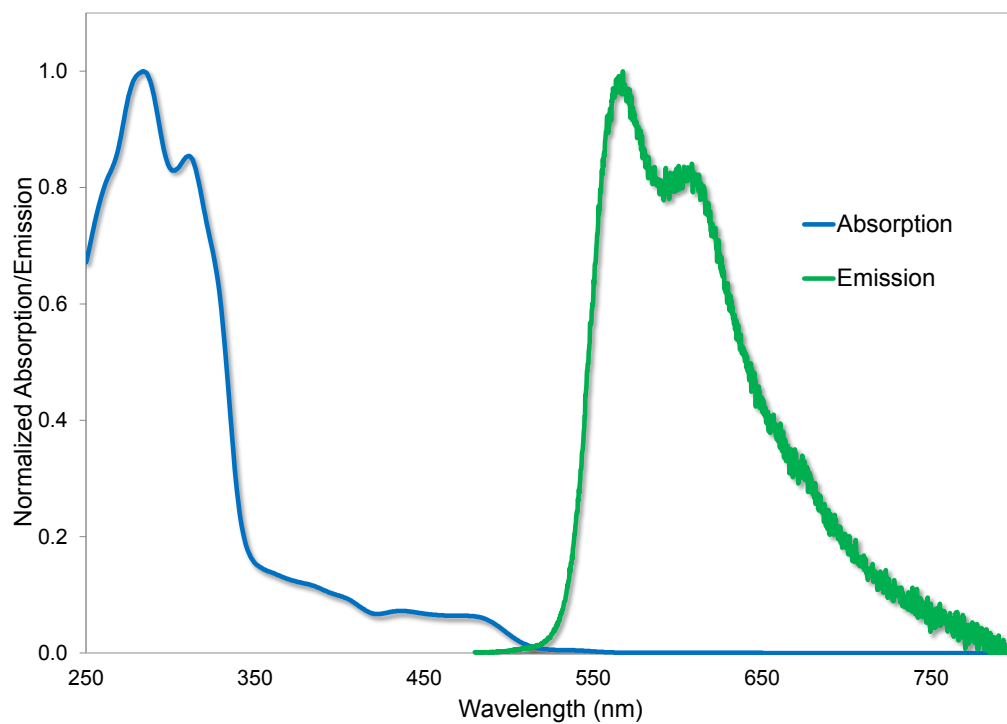


Figure S23. Normalized absorption and emission spectra of complex **1a**.

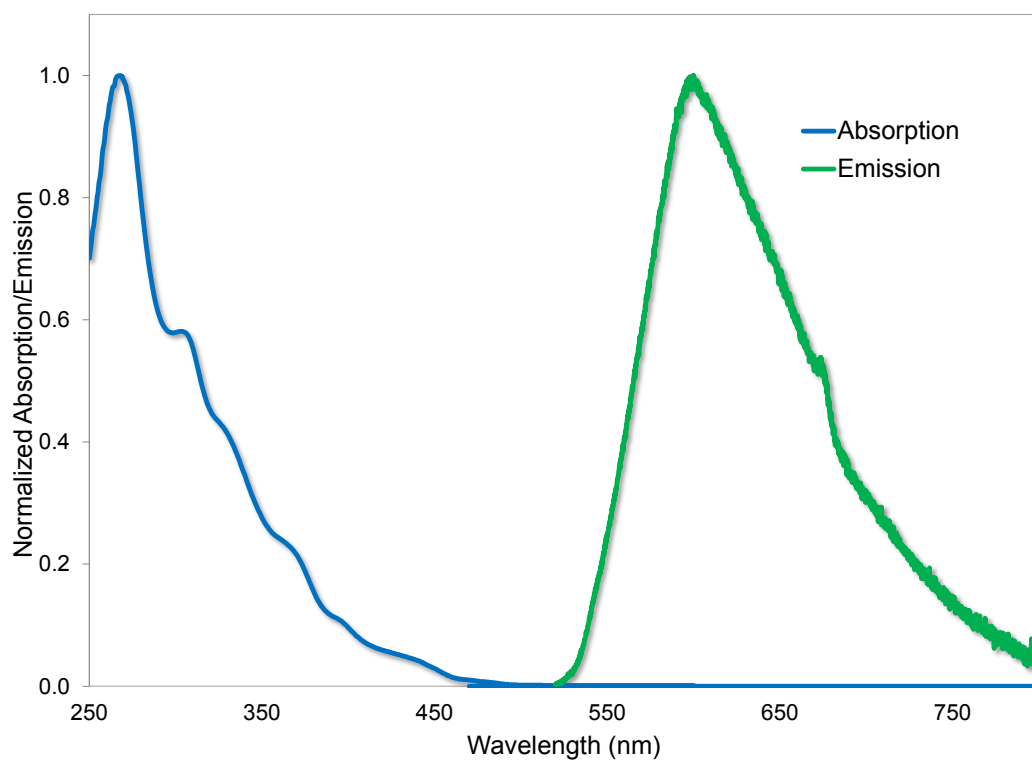


Figure S24. Normalized absorption and emission spectra of complex **1b**.

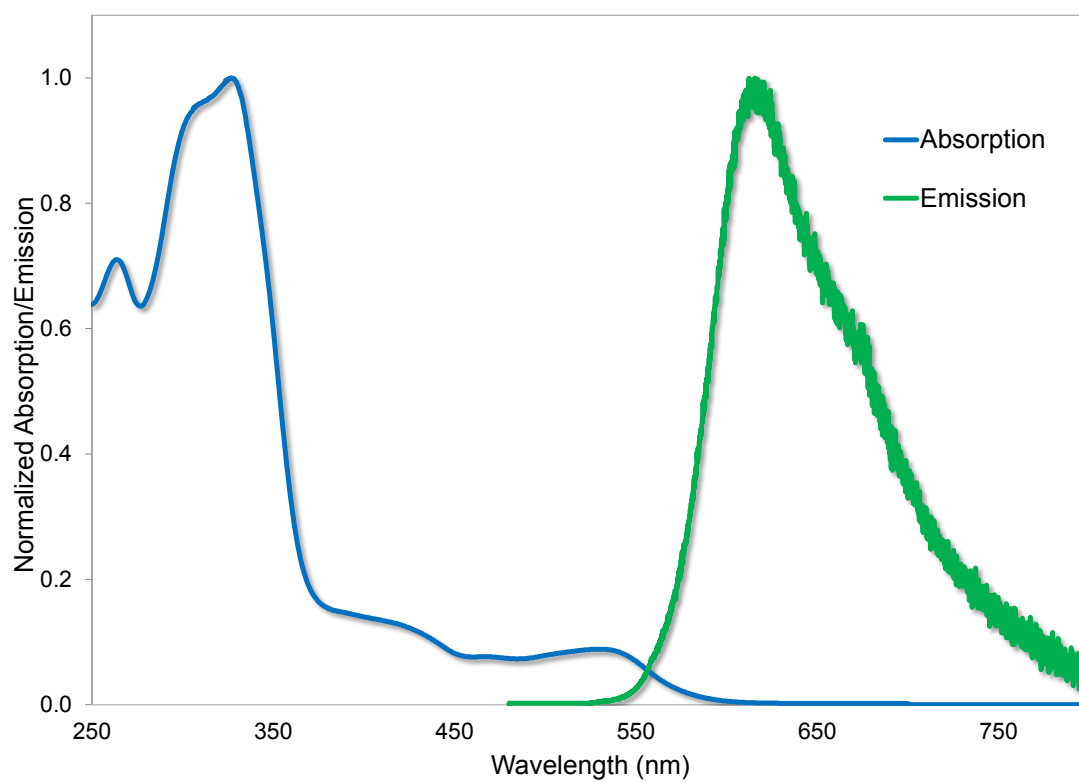


Figure S25. Normalized absorption and emission spectra of complex **2a**.

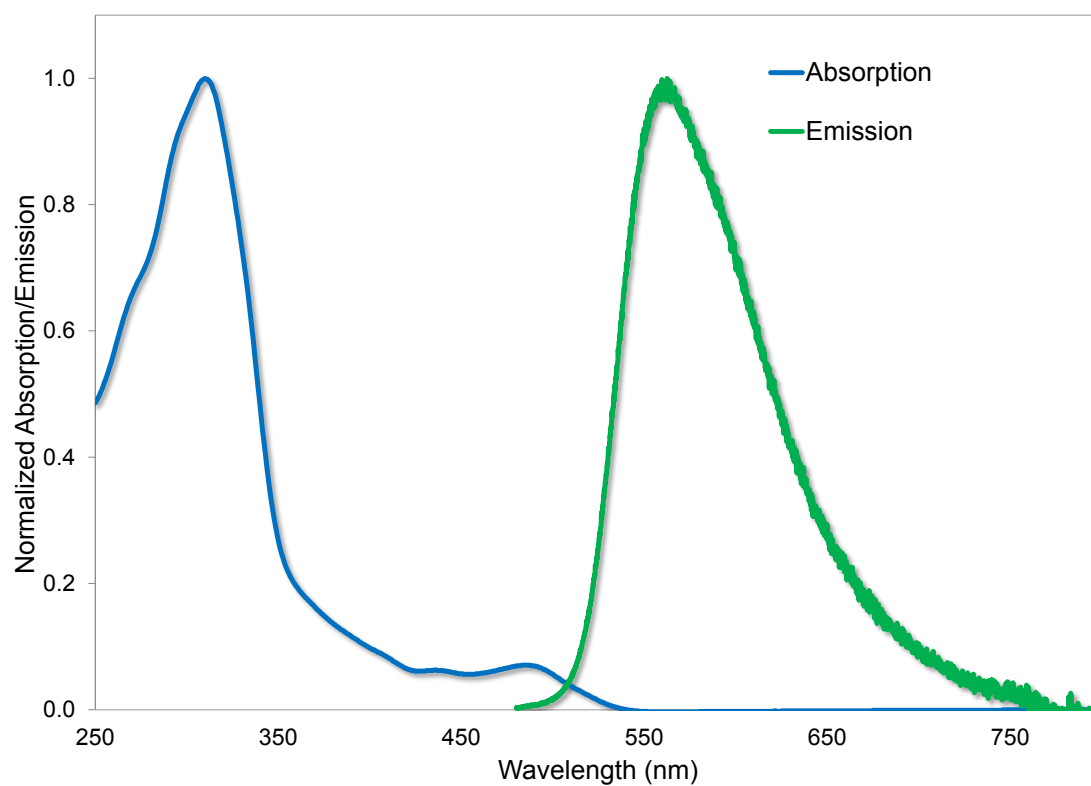


Figure S26. Normalized absorption and emission spectra of complex **2b**.

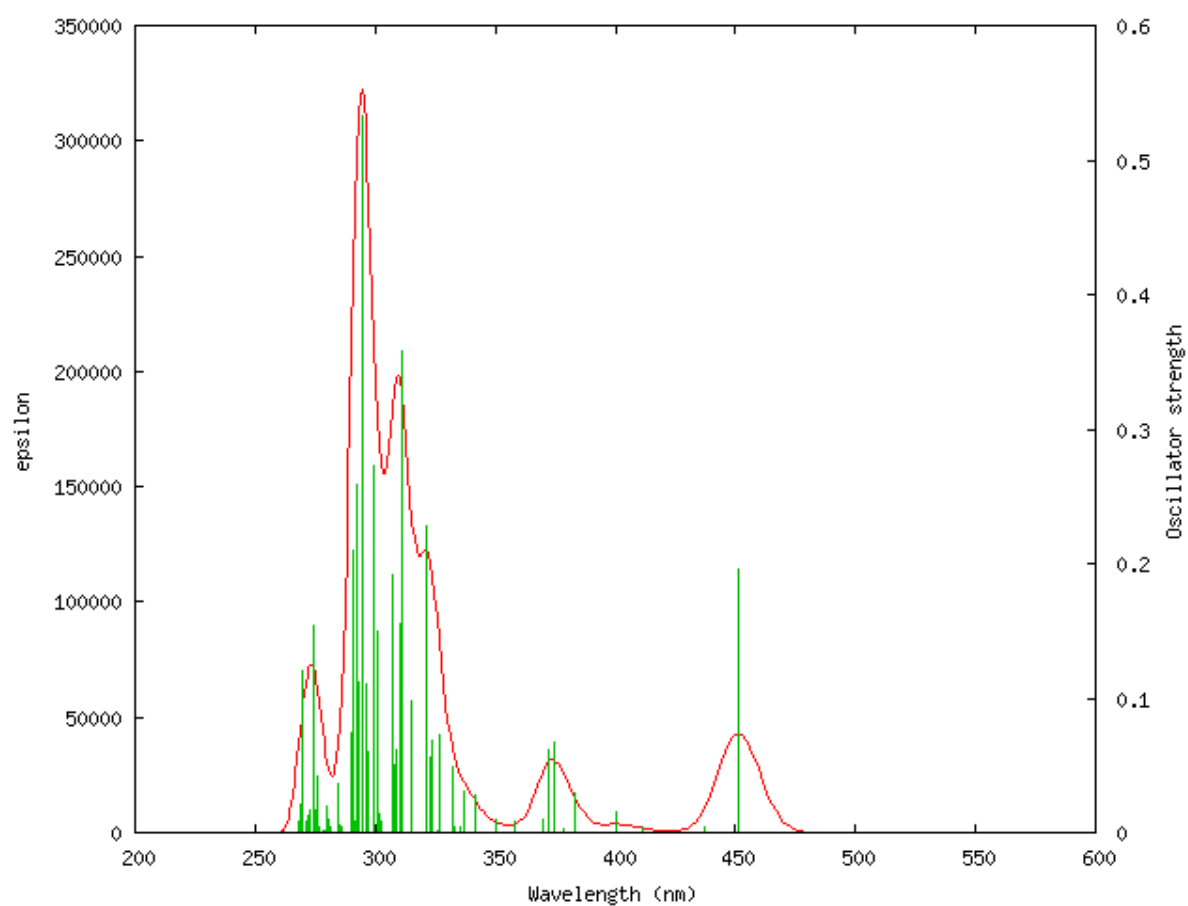


Figure S27. Calculated absorption spectra for **1a**

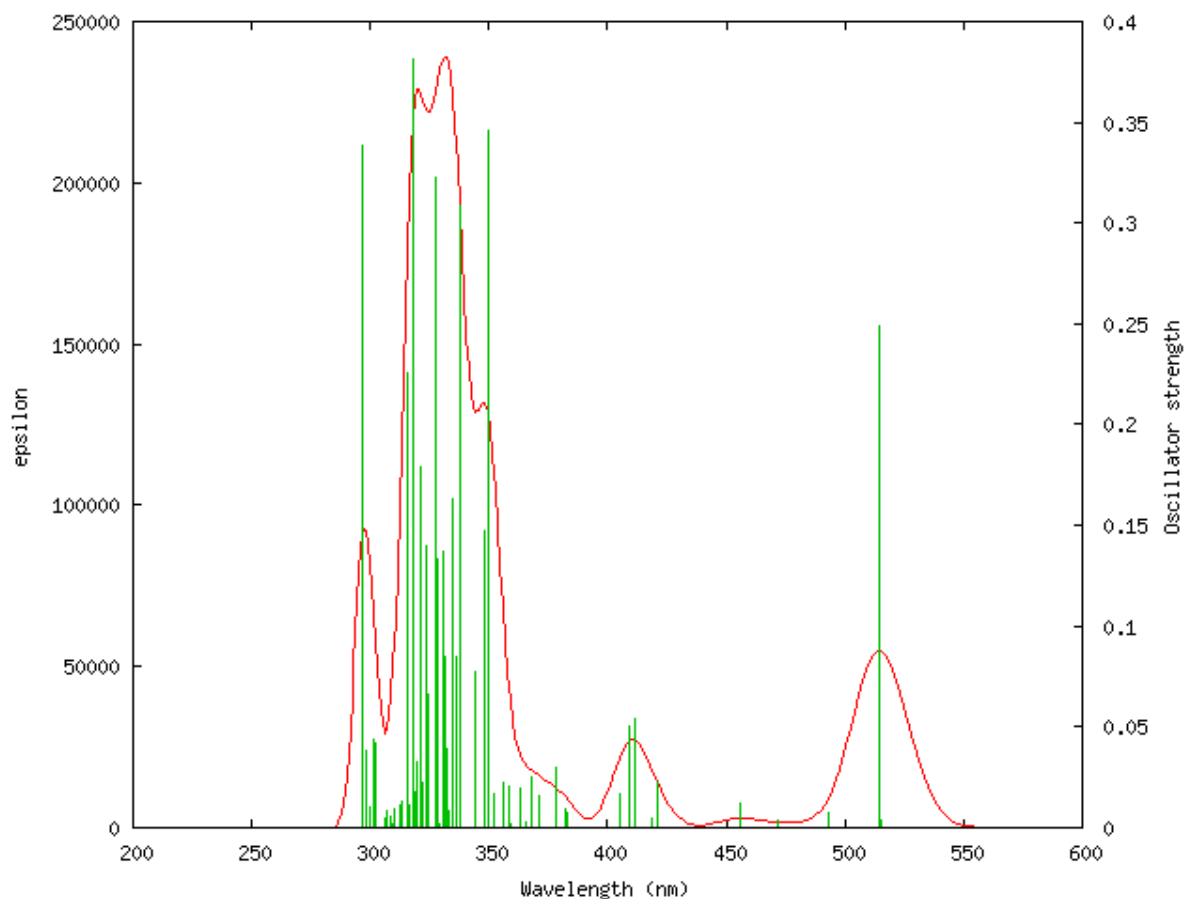


Figure S28. Calculated absorption spectra for **2a**

Table S1. Relevant absorption data for **1a-2b**

| Complex                                    | $\lambda_{\text{abs}}/\text{nm}$ ( $\epsilon \times 10^4 / \text{M}^{-1} \text{cm}^{-1}$ )     | $E_{0,0}$ (eV) |
|--|--|----------------|
| <b>[Ir(ppy)<sub>2</sub>Cl]<sub>2</sub></b> | 261 (8.00), 281 (5.00), 303 (3.12), 338 (1.35), 356 (1.10), 403 (0.66), 454 (0.40), 481 (0.11) | 2.49           |
| <b>1a</b>                                  | 284 (8.12), 309 (6.92), 330 (4.81), 381 (0.97), 406 (0.76), 485 (0.50)                         | 2.38           |
| <b>1b</b>                                  | 267 (7.60), 304 (4.31), 328 (3.22), 368 (1.70), 397 (0.73), 445(0.32), 468 (0.07)              | 2.58           |
| <b>2a</b>                                  | 264 (5.33), 300 (6.92), 327 (7.61), 350sh (4.49), 427 (0.88), 539 (0.65)                       | 2.10           |
| <b>2b</b>                                  | 268 (6.21), 311 (9.78), 336 (5.75), 410sh (0.84), 437 (0.65), 485 (0.70)                       | 2.33           |



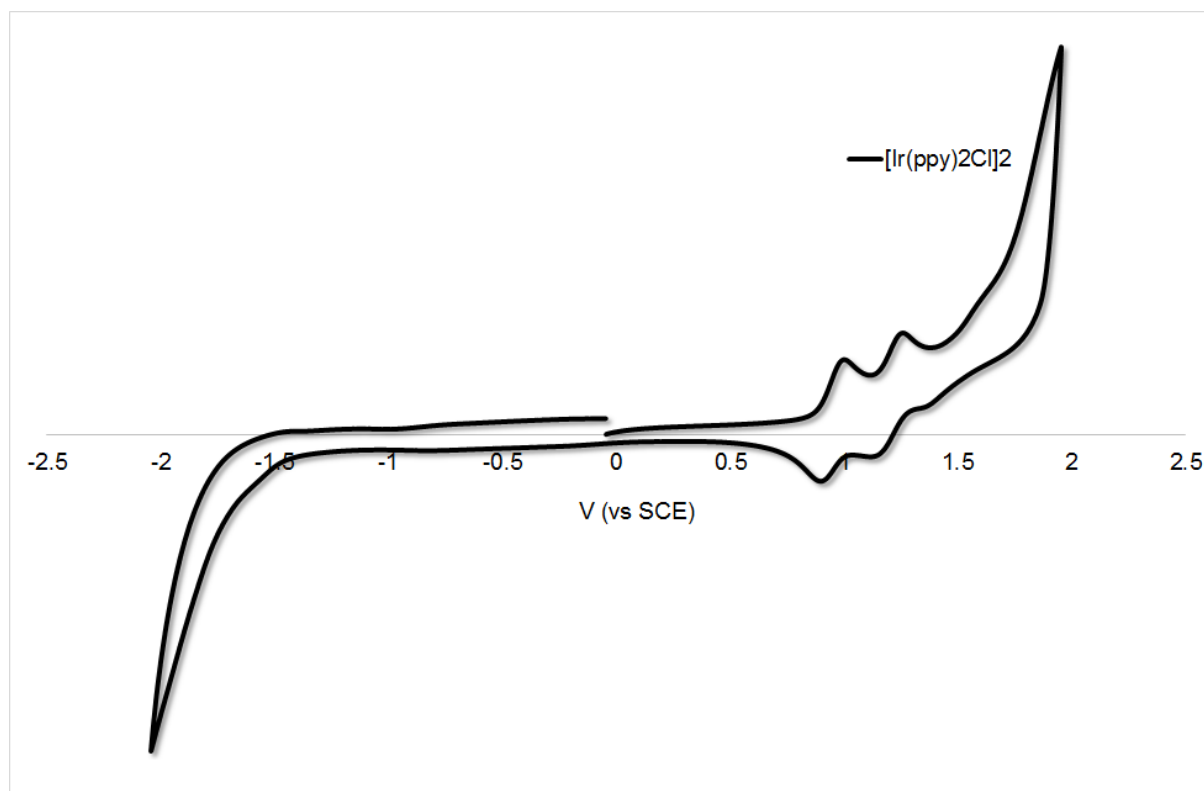


Figure S29. CV trace of complex  $[\text{Ir}(\text{ppy})_2\text{Cl}]_2$ .

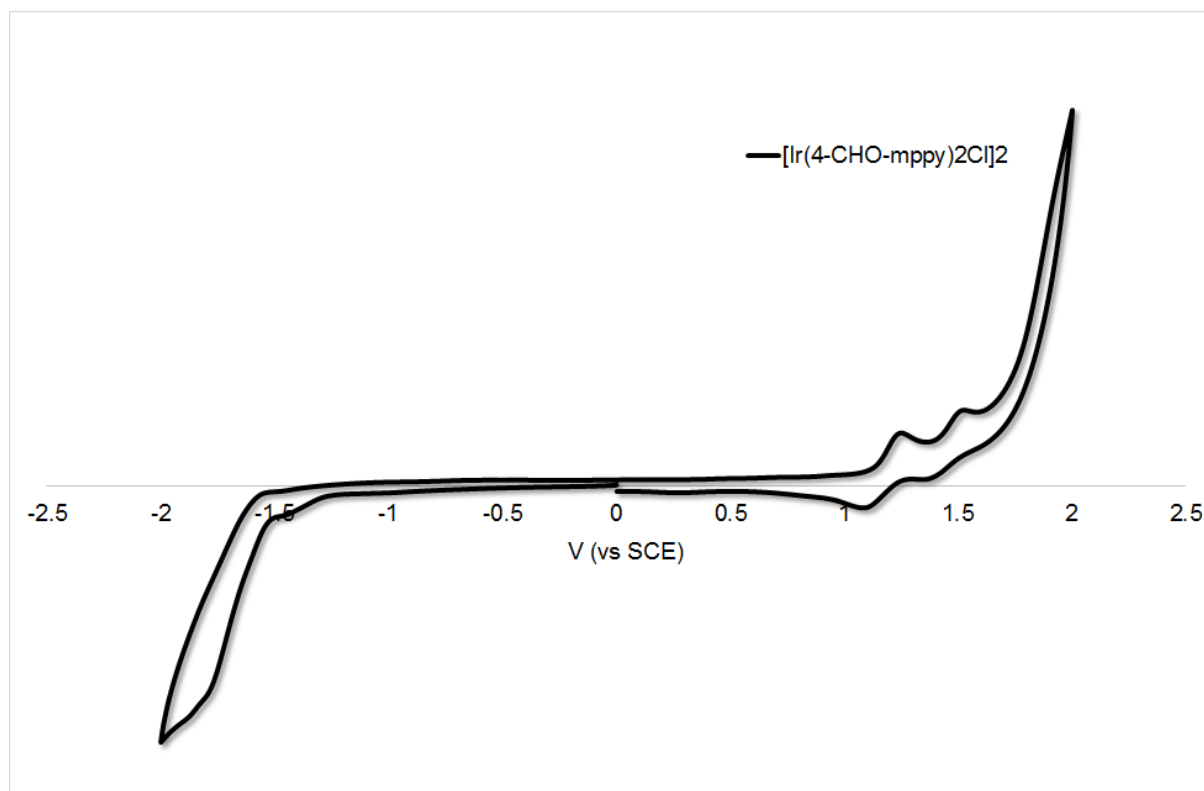


Figure S30. CV trace of complex **1a**  $[\text{Ir}(4\text{-CHOmpy})_2\text{Cl}]_2$ .

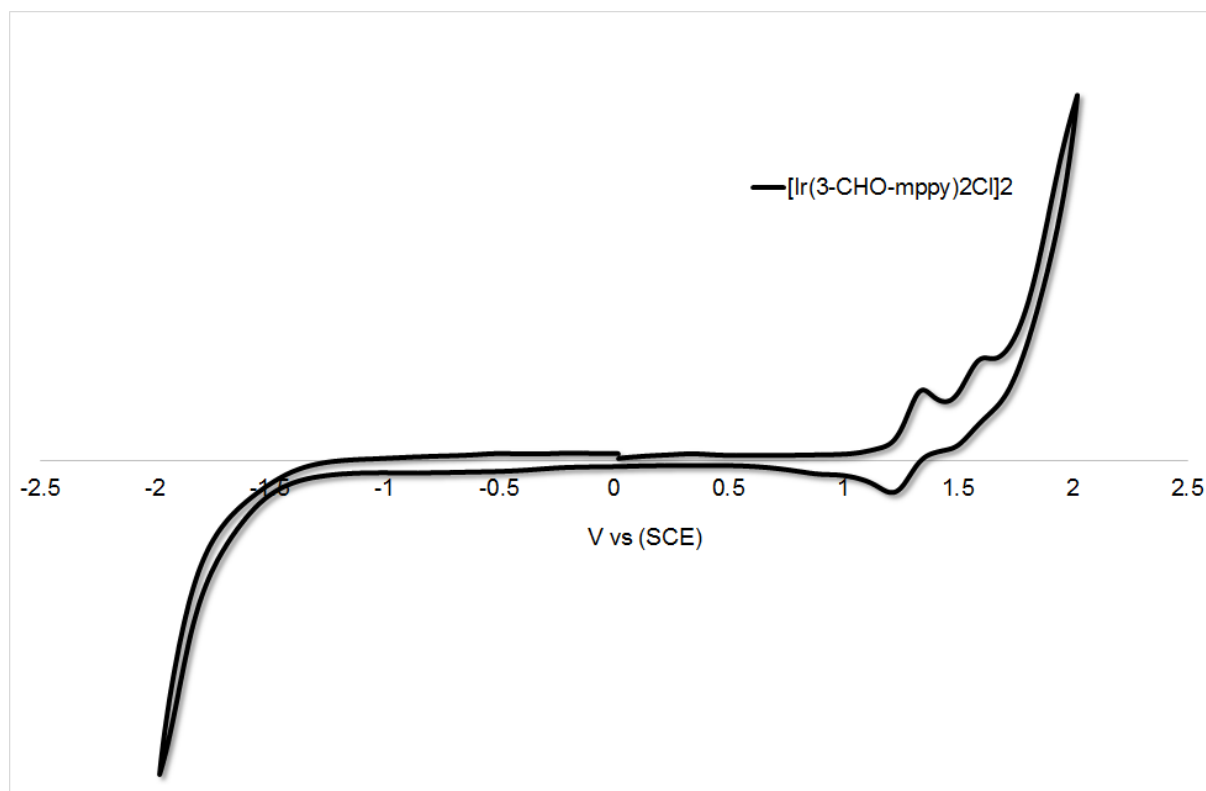


Figure S31. CV trace of complex **1b**  $[\text{Ir}(\text{3-CHOmppy})_2\text{Cl}]_2$ .

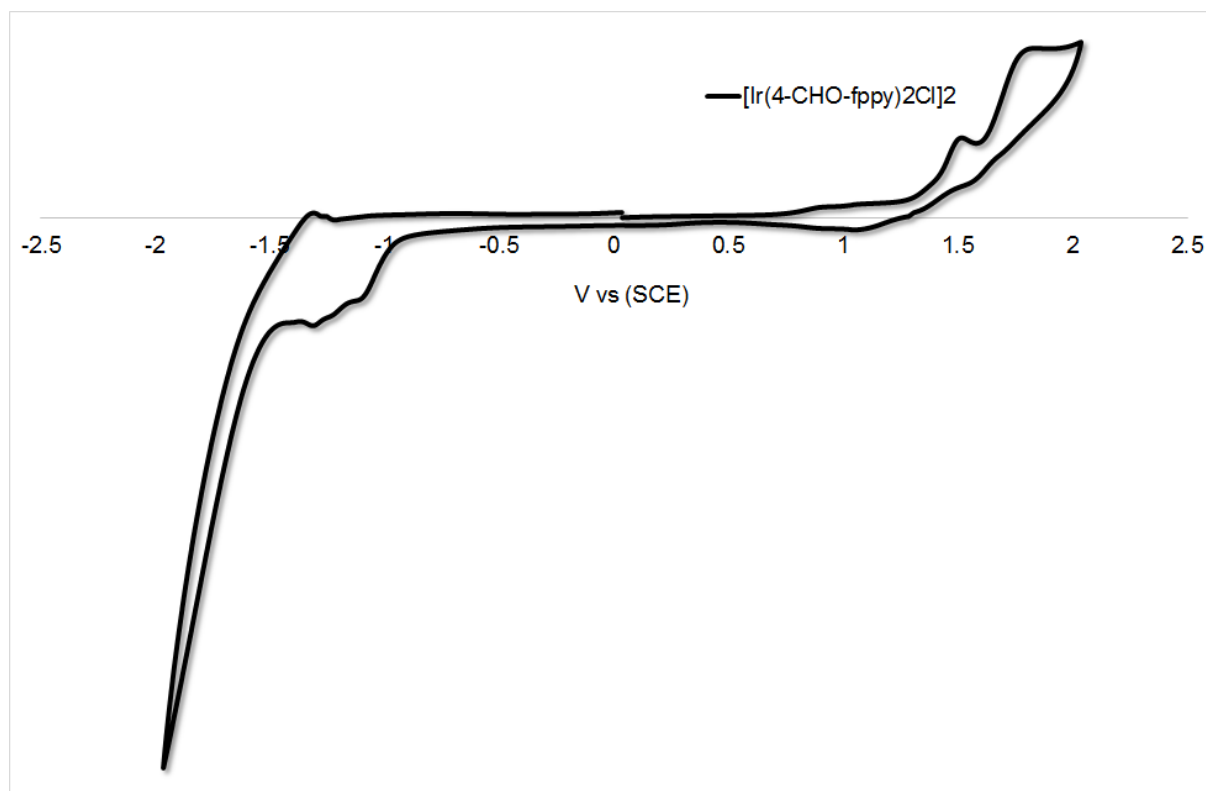


Figure S32. CV trace of complex **2a**  $[\text{Ir}(\text{4-CHO-fppy})_2\text{Cl}]_2$ .

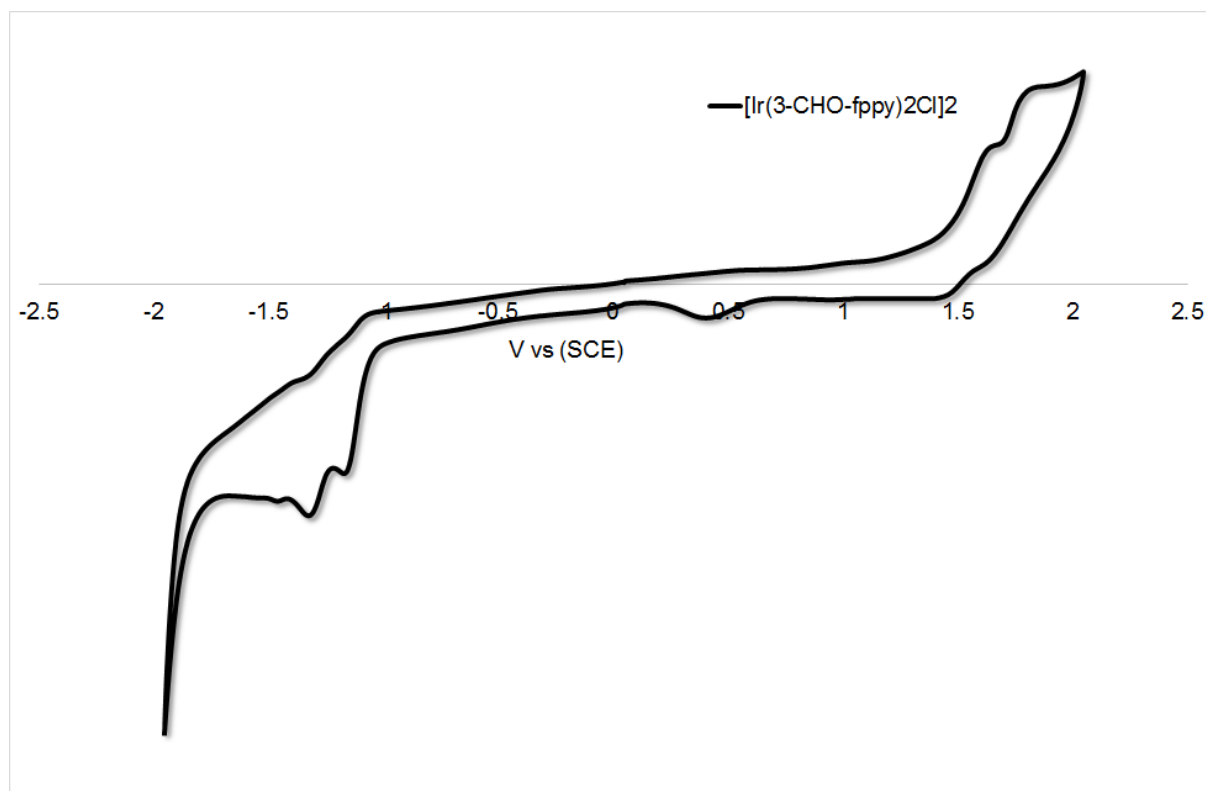


Figure S33. CV trace of complex **2b**  $[\text{Ir}(\text{3-CHO-fppy})_2\text{Cl}]_2$ .